NUMERICAL SIMULATION OF EFFECTS OF VELOCITY AND DIFFUSION COEFFICIENT ON CONCENTRATION OF CONTAMINANTS IN FLUID FLOW

BY

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR MASTER OF SCIENCE DEGREE IN APPLIED MATHEMATICS IN SCHOOL OF SCIENCE OF UNIVERSITY OF ELDORET, KENYA

JANUARY, 2022

DECLARATION

Declaration by the student

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DEDICATION

I devote my thesis to my wife Linda Langat for her support, love and prayers. I also earmark this thesis to my son Kiprop Mark Ngetich, my father Robert koech, my mother Pauline Koech, my brothers Shadrack's family, Peter's family, Weldon's family, Philemon's family, my only sister Stella's family, Rev. Reuben Koech's family, Mr. Albert Bii, and all staffs University of Eldoret Mathematics and Computer Science department, Kaplong Boys and Sikawa Secondary School staffs for the support and cooperation they gave me throughout my research .To my great loving family of Dr.Muruka and her loving wife Dr. Daisy Ruto, in-laws and friends who gave valuable comments during my study.

ABSTRACT

The study developed and implemented Implicit and explicit schemes for solving one dimensional convection –diffusion equation modeling concentration of contaminant in a fluid flow .The study uses method of lines and exact method to further verify the numerical solution obtained. Stability of the scheme was analyzed and accuracy of the solution to the contaminant transport equation was validated by exact solution. Graphical illustration of the solution for varying velocity and diffusion coefficient is given, Errors in the methods tabulated. The explicit method (EM) involved one unknown on left hand side (LHS) of the scheme while implicit method (IM) involved several unknowns on LHS of the scheme and method of lines (MOL) involved semi-discretization method. In the study, we examined effect of velocity and diffusion coefficient on concentration of contaminant in a fluid flowing .Comparison of solution from the methods stated was done. The developed, numerical schemes were developed and MATLAB used generate and in analyze the results. The results showed that concentration of contaminants increased inversely with fluid velocity and directly with diffusion coefficient. Therefore, for proper treatment of water for example, it is necessary to increase the flow velocities to reduce the concentration of contaminants. The implicit Method significantly agreed to exact method to three decimals than the explicit method which was much more inaccurate because of unconditional stability. As Velocity increases the concentration of contaminant decreases and as diffusion coefficient increases the concentration of contaminant increases.

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LIST OF ABBREVIATIONS, ACRONYMS AND SYMBOLS

C_{xx}	Second spatial derivative of concentration
C_x	First spatial derivative of concentration
μ	Velocity of flow
1D	One Dimensional
ADE	Advection-Diffusion Equation
BCs	Boundary conditions
BDS	Backward Difference Scheme
C	Concentration (dependent variable)
CDE	Convection-Diffusion Equation
CDS	Central Difference Scheme
CNM	Crank-Nicolson method
C_t	Time derivative of concentration
D	Diffusion constant
EM	Explicit method
EXACT SOL	Exact solution
FDA	Finite Difference Approximation
FDE	Forward Difference Scheme
ICs	Initial conditions
IM	Implicit Method
L	Length of channel (independent variable) in meters
LHS	Left hand side
MATLAB	Matrix Laboratory

MOL	Method of lines
ODE	Ordinary Differential Equation
Ode45	Ordinary Differential Equation uses fourth and fifth order Runge – kutta Algorithms
PDE	Partial Differential Equation
RHS	Right hand side
T	Simulation time in seconds
x, t	Independent variable
α	is the courant constant
β	is the ratio of stability
o	Order of error

ACKNOWLEDGMENT

I thank God for his unspeakable joy and grace that has enabled me to carry out this study. My appreciation goes to my supervisors: Prof Jacob Bitok and Dr Julius shichkha who worked tirelessly with me, giving valuable comments and positive suggestions that have enhanced the quality of this study. I would also like to thank the entire department of Mathematics and Computer Science of University of Eldoret particularly the Head Dr.Argwings Otieno Ranyimbo and Dean school of science Prof Lutta for their administrative support during my study period. My sincere regards also goes to my family members for their prayers, caring, loving, support and encouraging me to finish my studies. Finally to those who directly or indirectly contributed to the success of this work; May the glory of God richly bless you.

CHAPTER ONE

INTRODUCTION

1.1 Background information

Numerical simulations of partial differential equations (PDE) is of significance to environmentalists, hydrologist and mathematical modelers of real life application. This is to address current situation and problem solving approaches in science and engineering. The process of simulating this equations by numerical discretization based method for example finite difference method (FDM) become a greater point of concern due to computation, time and complexity of the methods used to solve convection-diffusion equation. The convection-diffusion equation (CDE) is a parabolic partial differential equation combining the diffusion and advection terms. Most problem on CDE occurs frequently in transport of ground water pollutants. Given Mass, momentum and heat are fundamental transfer phenomena in the universe and inside a physical system due to two process namely diffusion and convection, whereby diffusion is the spread of particles from a region of high to low concentration and convection is the movement of particles within fluids due to physical movement of the fluid. Numerical research focus on the study of the factors that affect the concentration of contaminant in the fluid flow like flow velocity and diffusion coefficient. This thesis is organized as follow: In chapter 2 literature review on the research done by various authors on solving CDE problems and the methods used. In chapter 3, the CDE are introduced with methods used to solve the equation under the study model. Chapter 4 deals with the analysis of the study basing on objectives set. Lastly, a summary of the results and the effect of velocity and diffusion coefficient on concentration of contaminant is in chapter 5.

1.2 Mathematical model of CDE

The mathematical model consider one dimension time dependent convection-diffusion equation with velocity and diffusion coefficient to be varied with assumption that velocity and diffusion coefficient are positive, for a general scalar variable and subjected to appropriate initial and Dirichlet boundary condition given by

$$C_t + \mu C_x = DC_{xx} \qquad 0 \leq x \leq L, \quad 0 \leq t \leq T \quad \ldots\ldots (1.1)$$

The exact method of equation (1.1) was derived by Dehghan (2005) as

$$C(x,t) = \sqrt{\frac{20}{t+20}}\, exp\left(\frac{-(x-2-\mu t)^2}{4D(t+20)}\right) \quad \ldots\ldots (1.2a)$$

$$c(x,t) = \sqrt{\frac{20}{t+20}}\, exp\left(\frac{-(x^2-4x-2x\mu t+4\mu t+\mu^2 t^2+4)}{4D(t+20)}\right) \quad \ldots\ldots (1.2b)$$

The solution of equation (1.2a) was used to obtain analytical solution and derived the initial and boundary conditions for our numerical study.

With initial condition,

$$c(x,0) = f(x) = exp\left(\frac{-(x-2)^2}{80D}\right) \qquad 0 \leq x \leq L \quad \ldots\ldots (1.3)$$

And Dirichlet boundary conditions:

Left boundary condition,

$$c(0,t) = g_o(t) = \sqrt{\frac{20}{t+20}}\, exp\left(\frac{-(2+\mu t)^2}{4D(t+20)}\right) \qquad 0 \leq t \leq T \quad \ldots\ldots (1.4)$$

Right boundary condition,

$$c(0,t) = g_L(t) = \sqrt{\frac{20}{t+20}}\, exp\left(\frac{-(1+\mu t)^2}{4D(t+20)}\right) \qquad 0 \leq t \leq T \quad \ldots\ldots (1.5)$$

Where the function f(x), $g_o(t)$ and $g_L(t)$ are known. The function values of C(x, t) are to be determined and used to validate the methods used with the assumption that the constants μ and D are positive and parameters to be investigated

1.3 Numerical schemes

The section presents the formulation of the three numerical schemes to CDE using FDM compare with exact method

1.3.1 Scheme 1: Implicit Backward Euler method

A difference schemes is implicit if the several unknown values can be expressed in terms of the known values. Generally we can express Crank-Nicolson method that space derivative is averaged.

$$\frac{c_{i,j+1} - c_{i,j}}{\Delta t} = \frac{D}{2}\left(\frac{c_{i+1,j+1} - 2c_{i,j+1} + c_{i-1,j+1}}{\Delta x^2} + \frac{c_{i+1,j} - 2c_{i,j} + c_{i-1,j}}{\Delta x^2}\right) + \frac{\mu}{2}\left(\frac{c_{i+1,j+1} - c_{i-1,j+1}}{\Delta x} + \frac{c_{i+1,j} - C_{i-1,j}}{\Delta x}\right)$$
…………………………………………………………………………........... (1.6)

1.3.2 Scheme 2: Explicit method scheme

A difference scheme is explicit if one unknown value can be expressed in terms of the known values. The time derivative is replace by forward differences, the first order partial derivative and the second order partial derivative of concentration to respect to x both replaced by central differences approximation.

$$\frac{c_{i,j+1} - c_{i,j}}{\Delta t} ++ \mu\left(\frac{c_{i,j+1} - c_{i-1,j}}{\Delta x}\right) = D\left(\frac{c_{i+1,j+1} - 2c_{i,j} + c_{i-1,j}}{\Delta x^2}\right)$$
.... (1.7)

1.3.3: Method of lines scheme

Method of lines is a semi discretization technique in which only the spatial derivative is discretized.

This gives rise to systems of ODE from where we can employ ODE solvers like Ode45.

1.4: Dimension of a PDE

The dimension of a PDE is the number of the spatial variables. Hoffmann (2000)

For example

(i) $C_t = C_{xx}$ is 1D because it has space variable x only …………………… (1.8a)

(ii) $C_t = C_{yy} + C_{xx}$ is 2D because it has the variable x and y ……..…………… (1.8b)

1.5: Classification of a PDE

Hoffmann (2000);The PDE can be classified into three namely

(i) Parabolic PDE

$$C_t = C_{xx} \qquad (1.9a)$$

(ii) Elliptic PDE

$$C_{xx} + C_{yy} = 0 \qquad (1.9b)$$

(iii) Hyperbolic PDE

$$C_{tt} = C_{xx} + C_{yy} \qquad (1.9c)$$

1.6. Basics of Finite Difference Methods (FDM)

This method is based on Taylor Series. We have Forward, Backward and Central difference approximations of derivatives. Hoffmann (2000);

For ordinary derivatives, we have

(i) Forward difference

$$\frac{dC}{dx} = \frac{C_{(j+1)} - C_j}{\Delta x} + o\,(h) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.2)}$$

(ii) Backward difference

$$\frac{dC}{dx} = \frac{C_j - C_{j-1}}{\Delta x} + \text{o (h)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.3)}$$

(iii) Central difference

$$\frac{dC}{dx} = \frac{C_{j+1} - C_{i-1}}{2\Delta x} + \text{o (h)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.4)}$$

For partial derivatives, we have

$$C_x = \frac{C_{i+1,j} - C_{i,j}}{\Delta x} + o\,(h) \quad \text{(Forward in x)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.4)}$$

$$C_{xx} = \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{\Delta x^2} + o(h^2) \quad \text{(Central in x)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.5)}$$

$$C_t = \frac{C_{i,j+1} - C_{i,j}}{\Delta t} + o\,(h) \quad \text{(Forward in t)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.6)}$$

$$C_t = \frac{C_{i,j} - C_{i,j-1}}{\Delta t} + o\,(h) \quad \text{(Backward in t)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(1.9.7)}$$

The j is the subscript of time interval where i is subscript of x internal.

Where o(h) is the first order and $o(h^2)$ is the second order, $o(h^n)$ for n = 1, 2,…… n+1 which are the order of error.

1.7: Basic definitions of fluid flow

Wei (2016); Laminar flow is a type of flow in which the fluid particles move along streamline and all streamline are straight and parallel and also Reynolds number is less than 2000.

Turbulent flow is a type of flow in which the fluid particles move in zigzag way and also Reynolds number is more than 4000.

Steady flow is a type of flow in which the fluid at a given point do not change with time.

Unsteady flow –Is the type of flow where the fluid properties (mass, volume, density, temperature and pressure) at a point changes with time.

1.8: Statement of the problem

To study the effects of velocity and diffusion coefficient on concentration of contaminant through porous medium by numerically solving the parabolic partial differential equation using finite difference approximation (FDA). Convection diffusion transport problems arises in several area of science and engineering. This problem occur frequently in the transport of pollutants in ground water. Pollutants are unwanted materials in a substance that can cause harm to human health and contaminants are inputs of alien and potentially toxic substances into the environment for example untreated sewage discharge.

1.9: General objective

The general objective of the study was to analyze the effect of flow velocity and diffusion coefficient on concentration of contaminants in ground water using numerical simulation model.

1.9.1. Specific objectives

The specific objectives are:

1. To analyze effect of velocity on the concentration of contaminant.

2. To analyze effect of diffusion coefficient on the concentration of contaminant.

3. To determine accuracy of the numerical methods.

1.10: Significance of the study

Detection of contaminants in fluid flow helps in treatment fluid flow in channel and improvement of the procedure used in treatment of water. The concentration of the contaminant will help us in the filtration and cleaning of the fluid.

1.11: Justification of the study

There is need for clean and uncontaminated water therefore, this study helps to determine the level of contamination

CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction

One convention diffusion equation have carried out by several environmentalists and mathematical modelers of real life application presented on their papers and reseach.

2.2 Literature review

Mojtabi, A and Deville, M (2015) studied a time dependent one dimensional linear advection – diffusion with Dirichlet homogenous boundary conditions with initial sine function using finite element method. They found that the analytical solution was harder to evaluate due advection become dominant. Hence they came up with an approach to solve it analytically thus the solution becomes ill behaved and harder to evaluate. They came up with an approach where the simple wave solution were decomposed with viscous perturbation.

Thongmoon, M and Mckibbin, R (2006) studied 1D advection -diffusion equation by using numerical methods of cubic splines to estimate first and second derivatives by two standards finite difference schemes. They found that finite difference methods gave better solution than the spline method hence finite difference method is the best method in numerical simulation.

Kumar A, et al (2010) in his study on one-dimensional advection-diffusion equation with temporally dependent diffusion coefficients found that solute dispersion parameter is time dependent while the flow domain transporting the solutes is uniform hence both parameters are time dependent. They found that concentration on position and tine is faster in decreasing dispersion.

In the paper (Volker, J and Petr, k, 2005). A comparison of spurious oscillation at layer diminishing (SOLD) method for convection equation solved numerically convection dominated CDE with popular streamline upwind/petrov-Galerkin (SUPG) stabilization at spurious oscillation at layers is stable and lead to optimal convergence of the discrete solution. The upwind method was always the best method on regular grids in a 2D domain using finite element.

Hussain A, et al (2020) studied numerical analysis of CDE using modified upwind approach in finite volume method. The method was based on the second-order formulation for the temporal approximation and upwind approach of the finite volume method was used for spatial interface approximation. Some numerical experiments were conducted to illustrate the performance of new numerical scheme for a convection–diffusion problem. For the phenomena of convection dominance and diffusion dominance, they developed a comparative study of this new upwind finite volume method with an existing upwind form and central difference scheme of the finite volume method. From the study, modified numerical scheme showed highly accurate results as compared to both numerical schemes.

In the paper Weixiang. C, et al (2016).Supercovergence of the direct discontinuous Galerkin (DDG) method for convection –diffusion equation prove that DDG solution is super convergent with an order k+2 to a particular projection of the exact solution.

Karahan (2008) studied one 1D advection–diffusion equation with FDM using spreadsheet simulation. By changing only, the values of weighted parameter on ADE model, solutions were obtained by Upwind and Lax–Wendroff schemes. It was determined that the Lax–Wendroff scheme is in good agreement with analytical solution, the results of the model may easily be analyzed graphically.

In the paper (Jinchao.x, et al, 1999) .A monotone finite element scheme for convention – diffusion equation. They show that edge – averaged finite element scheme by discretization of convection –dominated thus found that it is easy to analyze and suitable for problems with a relatively smooth flux variables.

Wei and Xu (2016) studied the integral equation approach to the unsteady CDE using the second order Adams-Moulton method. The study found the characteristic variation multiscale method and the finite volume element method, the integral equation approach shows a higher accuracy. Compared with the finite volume element method the integral equation approach has a better convergence. In solving the convection dominated convection-diffusion problems the integral equation approach demonstrates a good stability.

In the paper (Aswin et al, 2015) did a comparative study of numerical schemes for convection-diffusion equation using differential quadrature and finite difference. The first scheme that time derivative is approximated using forward difference and the space derivatives using polynomial based differential quadrature method and second scheme used discretization of time and space derivative are done. The study found that the numerical schemes are in excellent agreement with the exact solution.

Bellew,S and O'Riordan.E (2003) in their paper A parameter robust numerical method for a system of two singular perturbed convection- diffusion equation which involved an appropriate piecewise uniform shishikin mesh showed that converge to continuous solutions uniformly with respect to the two singular perturbation parameters.

Gurarslan et al (2013) studied the numerical solution of advection-diffusion equation using a sixth-order compact FDM using the combined technique instead of conventional solution techniques. The accuracy and validity of the numerical model was verified through the presented results and the literature. The computed results showed that the use of the current method in the simulation is very applicable for the solution of the advection-diffusion equation.

Munyakazi.J.B, (2010) on his paper a uniform convergent monstandard finite difference scheme for a system of convection –diffusion equations proved that underlying discrete operator satisfies a stability at maximum normal convergence rate is linear with respect to the step size.

Lorimer and Artymko (2019) studied the effect of velocity and diffusion functionality on nonlinear mass transfer of solvent oil recovery using FDM. The results obtained from this analysis indicate that functionalities determine the shape of the solvent concentration profile. Preliminary results from their study suggest that the velocity functionality has more influence on the process at both the lab and field scales for parameters considered in their study. The shapes of the concentration profiles were affected by both diffusion functionality and velocity functionality.

In the paper (Krukier, L.A, et al, 2013) Numerical solution of the steady convection-diffusion equation with dominant convection. They successfully presented and considered new class of product triangular skew symmetric iterative method for solution of system in 2D with numerical experiments using finite-difference approximation.

Logan and Zlotnik (1995) Studied convection-diffusion equation on semi-infinite domain with periodic Boundary condition .They show that the boundary condition took periodic concentration and a transformation thus obtained the same solution of two pure boundary value problem .They further found that boundary condition had single harmonic dependency on frequency, convection decay factors and diffusion.

Rizwan (1997) studied one-dimensional convection –Diffusion equation using second order space with time Nodal method. He solved numerical problems in steep concentration gradients for the one-dimensional convection –Diffusion equation. He found that the scheme was characterized by inherent numerical, examples show that the method used for solved problems in steep concentration gradients and small Peclet numbers by not introducing artificial viscosity without any sign of numerical dissipation.

Dehgham.M, (2005) studied convection –Diffusion Equation on one –dimension by the numerical solution .He found that the best and accurate method was the new fourth-order explicit formula. It was evident that the approach presented was naturally generalized to degree of finite difference method on linear dependent partial differential equation.

Evans and Abdullah (1985) studied convection diffusion equation by new explicit method where the schemes are develop a method called Group explicit method. They found that characteristics stability and capability solution were obtained on many points concurrently thus enabling the explicit method to compete with implicit methods on level terms. They further show that forward and backward differences were made of approximations thus being more tedious method. The approximations to $\partial u/\partial y$ on both forward and backward differences at different time level is always superior that the Crank-Nicolson up winding scheme where $\partial u/\partial x$ is always approximated by the backward difference.

Feng and Zheng (2009) studied Convection-diffusion equation in 1D using domain decomposition and alternating group to solve it. They found that methods used were more effective in convection dominant. They further applied concept of construction of the method to 2D convection diffusion equation and they summed up the methods and found that they have intrinsic parallelism and best on parallel computation.

Perez Guerrero (2009) studied analytically advection -diffusion transport using change of variable and integral transform technique for transient and steady state regimes with constant coefficient. They found that exact solution of the linear advection –dispersion transport equation were very advantageous on improving convergence of the series solution.

Mazeheri (2013) studied advection-diffusion equation in one dimension analytically of point sources on time dependent emission patterns using the constant velocity and diffusion coefficient. The results show that analytical solution provides accurate estimation of the concentration hence suitable in verifying the transport codes. The limitation of solution was only valid for constant parameter and not complies with spatial resolution.

Geiser (2007) analyzed solution for CDE reaction equation with different retardation factors and application in 2D and 3D for dispersion reaction equation using discretization and solver methods for solving it. He showed that the parameter of the equation and velocity field used input to set the different values.

Kumar et al (2010) considered analytical solution of 1D ADE with variable coefficients in a finite domain using finite domain using Laplace transformation techniques. They showed that temporal dependent dispersion along uniform flow through homogenous medium in which solute dispersion is assumed proportional to the square of its velocity.

Budd (1998) considered convection –diffusion equation using grid adaptation technique. They used singular perturbation and bifurcation technique for simulation of solution. They found spurious solutions using mesh method hence equidistribution did provide spurious solution on a fixed mesh.

Reza Mohammadi studied exponential B-spline solution of convection-diffusion equations with Dirichlet's tile boundary conditions using crank-Nicolson method .He used exponential B-spline functions in space integration. He showed that technique used were very best on nonlinear partial differential equations.

Angstmann (2016) studied numerical solution of ADE using discrete time random scheme. They considered a limit of a discrete stochastic process on time and space for non-linear advection-diffusion. They showed that discrete time random used to construct a numerical method for the solution of several non-linear advection diffusion partial differential equations.

Zhuang (2009) studied advection-diffusion equation using numerical methods for nonlinear source term on a finite domain by variable-order fractional. In their study they showed that type of fractional differential equation were able to describe heavy-tailed motions more accurately.

Feng and Zheng (2009) studied advection diffusion reaction problems using Runge-kutta chebyshev methods. He found that reaction terms were highly stiff than implicit-explicit Runge-kutta-chebyshev methods. Otherwise the explicit second order Rung-kutta -chebyshev method were the best method.

Rios (2015) studied one dimensional linear advection-diffusion equation using finite differences and linear finite elements method with Dirichlet boundary conditions and a sinusoidal initial condition. He found that the results would be used to analyze the pollutant concentration distribution domain, as long as the real condition can be adequate to the theoretical ones.

Golz (2001) studied the convection-diffusion equation using finite domain on time varying boundaries with Dirichlet condition. The approach yields finite geometry formulation closed Eigenvalues on Eigen function expansion.

Asan (2015) studied convection-diffusion equation using fourth order finite difference method. He developed various numerical techniques by second, third and fourth-order difference schemes in space and a first-order explicit scheme in time.

Authors used various methods to solve CDE .None of them analyzed the effects of velocity and diffusion coefficient using implicit method, explicit method and method of lines.

CHAPTER THREE

RESEARCH METHODOLOGY

3.1 Implicit backward Euler method

The Implicit Backward Euler method is the best method because of its unconditionally stable. The stability condition was derived by Dehghan (2005). Stability is ratio between the mesh sizes Δx and Δt beyond which the schemes will not hold.

Replacing equation (1.1) with partial derivative with respect to t with backward. First and second derivative with respect to x with central.

$$\frac{C_i^K - C_i^{k-1}}{\Delta t} = \frac{-\mu(C_{i+1}^k - C_{i-1}^k)}{2\Delta x} + \frac{D(C_{i-1}^k - 2C_i^k + C_{i+1}^k)}{(\Delta x)^2} \quad (3.1.1)$$

Where k is variable of time and i is variable in x

Multiply equation (3.1.1) on both sides by Δt

$$C_i^K - C_i^{k-1} = \frac{-\mu \Delta t(C_{i+1}^k - C_{i-1}^k)}{2\Delta x} + D\Delta t \frac{(C_{i-1}^k - 2C_i^k + C_{i+1}^k)}{(\Delta x)^2} \quad (3.1.2)$$

$$C_i^K - C_i^{k-1} = \frac{-\mu\Delta t}{2\Delta x}\left(C_{i+1}^k - C_{i-1}^k\right) + \frac{D\Delta t}{(\Delta x)^2}\left(C_{i-1}^k - 2C_i^k + C_{i+1}^k\right) \quad (3.1.3)$$

We define $\alpha = \frac{\mu\Delta t}{2\Delta x}$, $\beta = \frac{D\Delta t}{(\Delta x)^2}$ α and β are stability ratios

Replacing α and β in equation (3.1.3) gives

$$C_i^K - C_i^{k-1} = -\alpha\left(C_{i+1}^k - C_{i-1}^k\right) + \beta(C_{i-1}^k - 2C_i^k + C_{i+1}^k) \quad (3.1.4)$$

$$C_i^K - C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + 2\beta C_{i+1}^k \quad (3.1.5)$$

$$-C_i^{k-1} = -\alpha C_{i+1}^k + \alpha C_{i-1}^k + \beta C_{i-1}^k - 2\beta C_i^k + \beta C_{i+1}^k - C_i^K \quad (3.1.6)$$

Dividing equation (3.1.6) on both side by negative, we have

$$C_i^{k-1} = \alpha C_{i+1}^k - \alpha C_{i-1}^k - \beta C_{i-1}^k + 2\beta C_i^k - \beta C_{i+1}^k + C_i^K \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(3.1.7)}$$

$$C_i^{k-1} = -\alpha C_{i-1}^k - \beta C_{i-1}^k + C_i^k + 2\beta C_i^k + \alpha C_{i+1}^k - \beta C_{i+1}^k \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(3.1.8)}$$

Re-arranging equation (3.1.8) we get

$$C_i^{k-1} = -(\alpha + \beta) C_{i-1}^k + (1 + 2\beta) C_i^k + (\alpha - \beta) C_{i+1}^k \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(3.1.9)}$$

Equation (3.1.9) is the implicit scheme to be programmed. It is simplified version of equation (3.1.1).

3.2 Explicit method (EM)

The unknown $C_{i,j+1}$ is on the LHS alone and the knowns are on the RHS,

By discretizing the PDE in equation (1.1) approximated by the FDA as

$$\frac{C_{i,j+1}-C_{i,j}}{\Delta t} + \mu\frac{(C_{i-1,j} - C_{i+1,j})}{2\Delta x} = \frac{D(C_{i-1,j} - 2C_{i,j} + C_{i+1,j})}{(\Delta x)^2} \quad (3.2.1)$$

Multiply equation (3.2.1) on both sides by Δt

$$C_{i,j+1} - C_{i,j} + \mu\Delta t\frac{(C_{i-1,j} - C_{i+1,j})}{2\Delta x} = \frac{D\Delta t(C_{i-1,j} - 2C_{i,j} + C_{i+1,j})}{(\Delta x)^2} \quad (3.2.2)$$

$$C_{i,j+1} - C_{i,j} = -\frac{\mu\Delta t}{2\Delta x}\left(C_{i-1,j} - C_{i+1,j}\right) + \frac{D\Delta t}{(\Delta x)^2}\left(C_{i-1,j} - 2C_{i,j} + C_{i+1,j}\right) \quad (3.2.3)$$

$$C_{i,j+1} = -\frac{\mu\Delta t}{2\Delta x}\left(C_{i-1,j} - C_{i+1,j}\right) + \frac{D\Delta t}{(\Delta x)^2}\left(C_{i-1,j} - 2C_{i,j} + C_{i+1,j}\right) + C_{i,j} \quad (3.2.4)$$

We define $\alpha = \frac{\mu\Delta t}{2\Delta x}$, $\beta = \frac{D\Delta t}{(\Delta X)^2}$ α *and* β are stability ratios; Replacing equation (3.2.4) with stability ratios gives

$$C_{i,j+1} = -\alpha\left(C_{i-1,j} - C_{i+1,j}\right) + \beta\left(C_{i-1,j} - 2C_{i,j} + C_{i+1,j}\right) + C_{i,j} \quad (3.2.5)$$

$$C_{i,j+1} = -\alpha C_{i-1,j} + \alpha C_{i+1,j} + \beta C_{i-1,j} - 2\beta C_{i,j} + \beta C_{i+1,j} + C_{i,j} \quad (3.2.6)$$

$$C_{i,j+1} = -\alpha C_{i-1,j} + \beta C_{i-1,j} + C_{i,j} - 2\beta C_{i,j} + \alpha_1 C_{i+1,j} + \beta C_{i+1,j} \quad (3.2.7)$$

Re-arranging equation (3.2.7) we get

$$C_{i,j+1} = (\beta - \alpha)C_{i-1,j} + (1 - 2\beta)C_{i,j} + (\alpha + \beta)C_{i+1,j} \quad (3.2.8)$$

as the numerical scheme

Hindmarsh (1984) and Sousa (2003) showed that the condition for stability is

$\frac{2D\Delta t}{(\Delta x)^2} \leq 1$ and $(\frac{\mu\Delta t}{\Delta x})^2 \leq \frac{2D\Delta t}{(\Delta x)^2}$ …………………………………………..……………. (3.2.9)

$r_1 = 0.2$, $r_2 = 0.5$, $\Delta t = 0.05$, $\Delta x \leq 0.1$ Where D and μ are parameters to be examined effect of concentration of contaminants. r_1 *and* Δt were assumed, r_2 and Δx were calculated from equation (3.2.9).

3.3 Method Of Line, MOL

Method of lines uses semi – discretization .We discretize only the spatial variable x and have temporal variables t. This gives a system of ODEs used ODE solver ode45 which uses the fourth and fifth order Runge-kutta Algorithms. Rearranging equation (1.1) as

$C_t = -\mu C_x + DC_{xx}$

$\frac{dC_i}{dt} = \frac{-\mu}{2\Delta x}(C_{i+1} - C_{i-1}) + \frac{D}{(\Delta x)^2}(C_{i-1} - 2C_i + C_{i+1})$ ……………………………… (3.3.1)

We define $\alpha = \frac{-\mu}{2\Delta x}$, $\beta = \frac{D}{(\Delta x)^2}$

$\frac{dC_i}{dt} = \alpha(C_{i+1} - C_{i-1}) + \beta(C_{i-1} - 2C_i + C_{i+1})$ …………………………………… (3.3.2)

$\frac{dC_i}{dt} = \alpha C_{i+1} - \alpha C_{i-1} + \beta C_{i-1} - 2\beta C_i + \beta C_{i+1}$ ……………………………………. (3.3.3)

$\frac{dC_i}{dt} = -\alpha C_{i-1} + \beta C_{i-1} - 2\beta C_i + \alpha C_{i+1} + \beta C_{i+1}$ ……………………….…………… (3.3.4)

$\frac{dC_i}{dt} = (\beta - \alpha)C_{i-1} - 2\beta C_i + (\alpha + \beta)C_{i+1}$ ……………………….…………………… (3.3.5)

For i = 1, 2…n+1

C_0 And C_{n+1} are the boundary conditions. Values of C were obtained from ode45 solver.

CHAPTER FOUR

RESULTS AND DISCUSSION

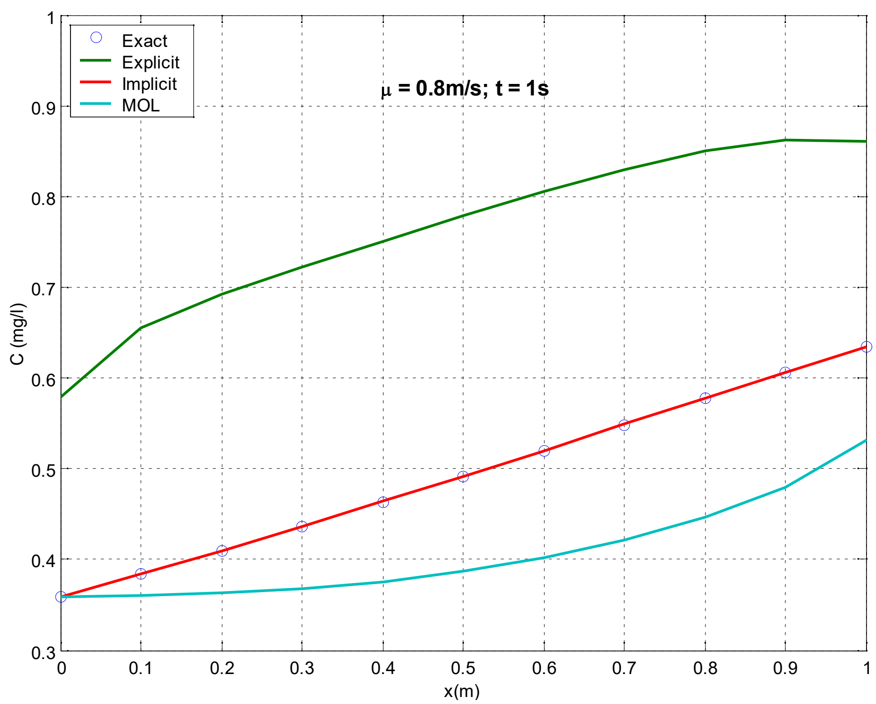
4.0 Introduction

This chapter presented schemes developed and solutions of schemes are discussed

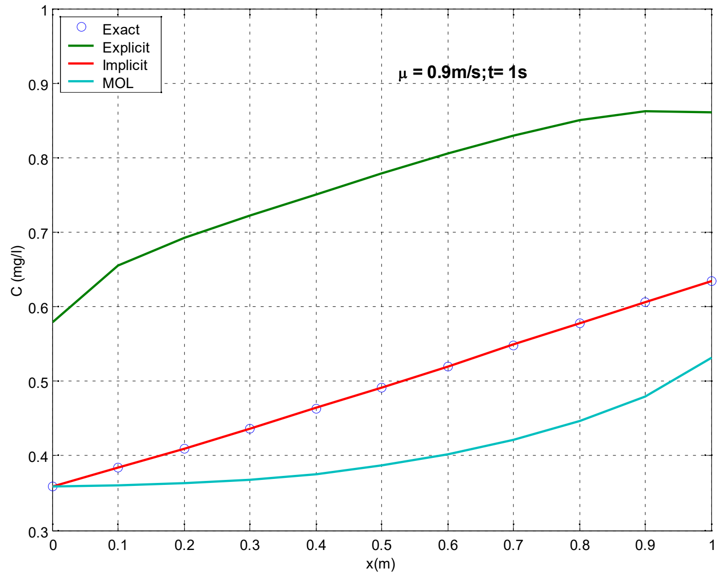
4.1 Results and discussion of objective 1

The variation of C (mg/l) with velocity when D = 0.1 at t = 1s are presented in figure 1 to analyze the effect of velocity on concentration of contaminant from data in table 1 of appendix 1.The numerical computations using uniform grid, for which a mesh of width $\Delta x = 0.1$m.

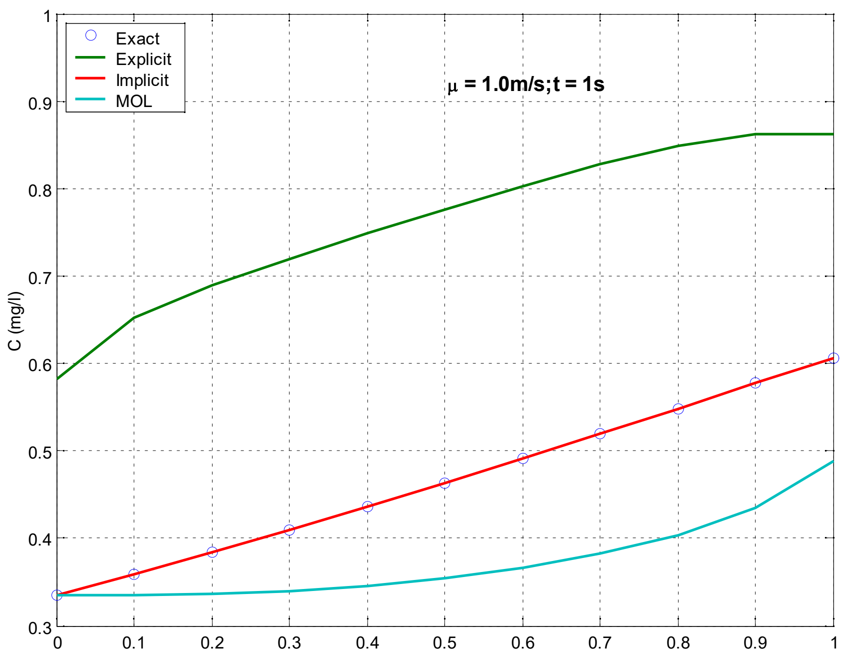
The results of scheme were generated using MATLAB in one-dimensional figures for the graphs and tables.



(a)



(b)



(c)

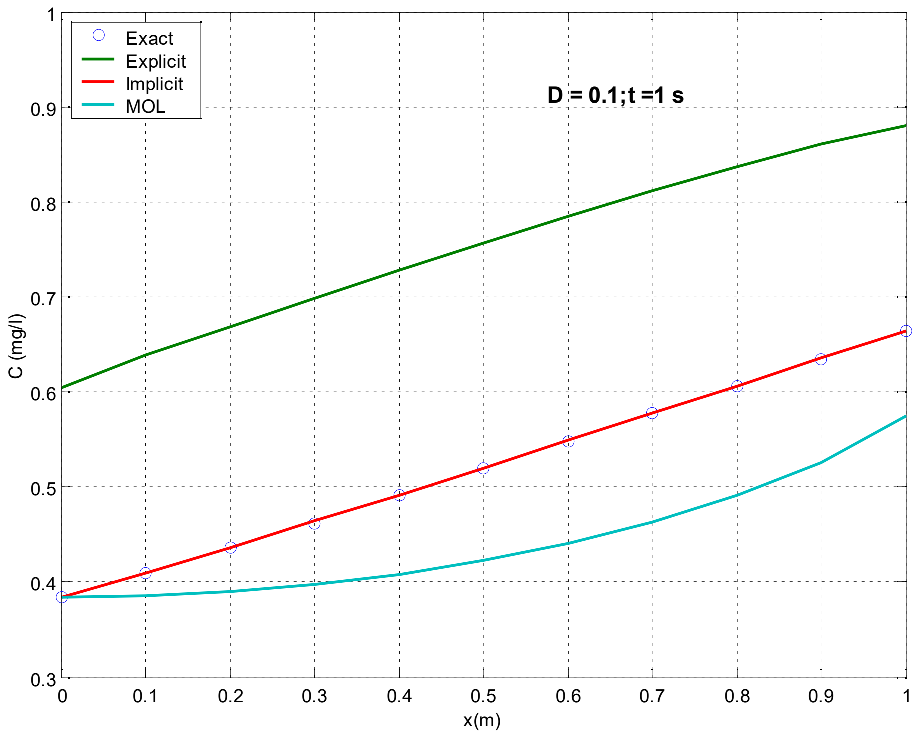
Figure 1: Comparison of methods of analysis at (a) μ=0.8 m/s (b) μ=0.9 m/s and μ=1 m/s at given constant time of 1s.

The figure 1 above clearly shows that as the values of flow velocity increases from 0.8 m/s to 1 m/s, the concentration of contaminants decreases. The Implicit and Exact schemes coincided linearly in the range of zero to one while MOL and Explicit schemes are nonlinear in the same range.MOL values of concentration contaminants clearly shows there is general nonlinear increases of concentration with decrease in velocity because of truncation errors due to discretization of space variable and also due to round off errors from solvers. The scheme portray smaller effects on concentration of contaminants as flow velocity increases compared to the other schemes. The curve is steeper at 0.8m that at 0.4m and the rate of change of concentration of contaminant with increases in flow velocity at figure 1c is higher than that at figure 1a.Implicit and exact schemes are approximately linear and portray that as flow velocity increases, the concentration of contaminants decreases. The rate of increase of concentration are nearly the same, take at x = 0.1m the difference rate of concentration of contaminant is 0.025mg/l (3dp).Explicit schemes values have higher effect of concentration of contaminants as flow velocity decreases compared to other schemes. From distance 0 to 0.1m, the concentration of contaminants has uniformly linear decreases as flow velocity increases while at distance 0.1m to 0.9m are linear in all figures than at 0.9m to 1m slightly bending without no effect of concentration of contaminants as flow velocity increases

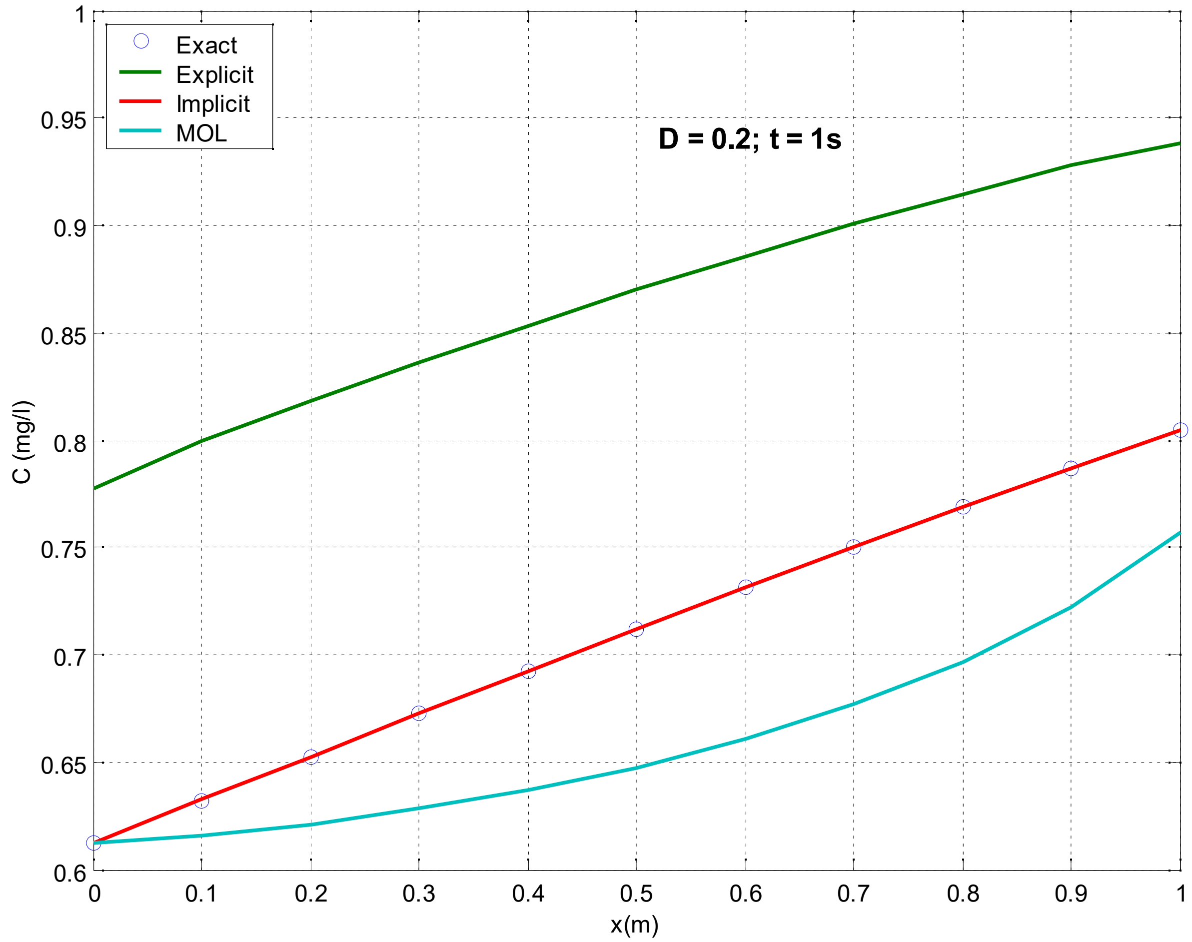
Generally above schemes shows that as the values of flow velocity increases from 0.8m/s to 1.0m/s, the concentration of contaminants decreases as D= 0.1 at 1s and also shows that smaller value of flow velocity has higher effect on concentration of contaminants.

4.2 Results and discussion of objective 2

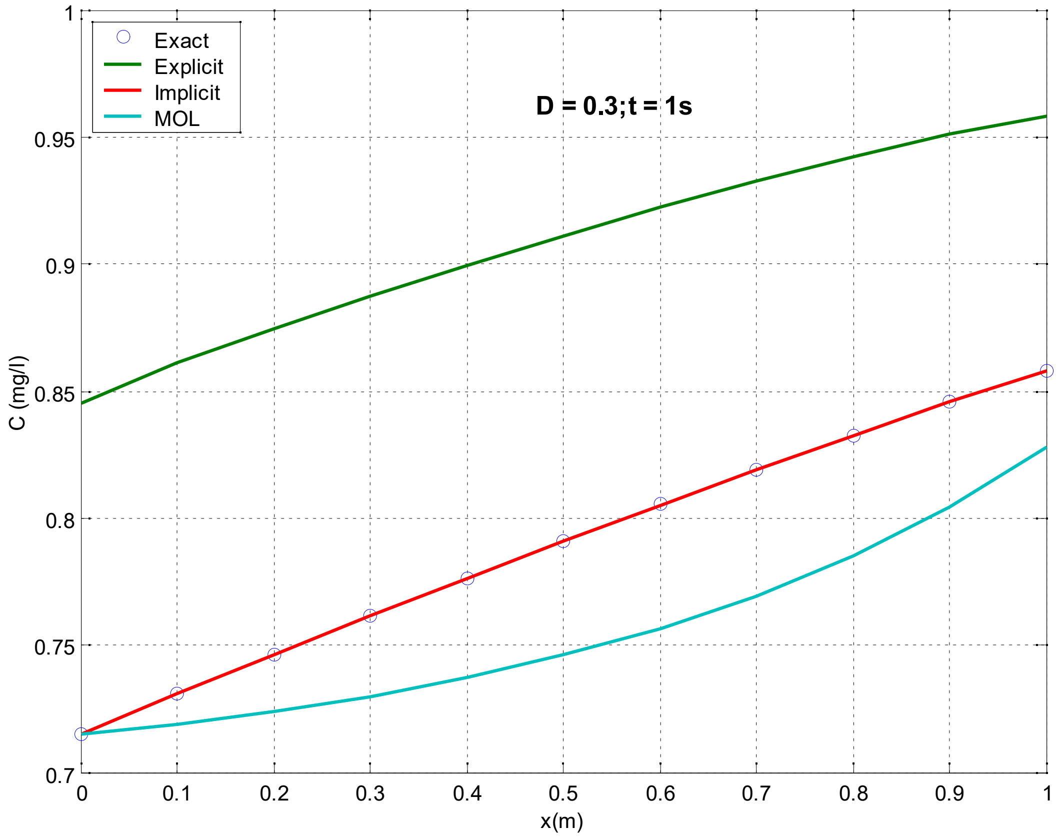
The results obtained using the exact method, implicit method, explicit method and method of lines on variation of C (mg/l) with diffusion coefficient when μ = 0.8 m/s at t = 1s are presented in fig. 2 to analyze the effect of diffusion coefficient on concentration of contaminants.



(a)


Exact
Explicit
Implicit
MOL
D = 0.2; t = 1s
C (mg/l)
x(m)
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

(b)



(c)

Figure 2: Effect of diffusion coefficient on concentration of contaminants using different methods at (a) D=0.1 (b) D=-0.2 and (c) 0.3 at constant time (1s) and constant velocity (μ=0.8 m/s)

The variation of diffusion coefficient keeping flow velocity constant $\mu = 0.8\ m/s$ at t = 1s from fig. 2 shows that implicit, explicit and exact scheme portray linear in the range of x from zero to one while MOL scheme is nonlinear in the same range.IM and Exact schemes coincided due to unconditionally stabilities from solver. At x = 0.5m C(x,t) = 0.5199,0.7123 and 0.7911 respectivity is directly proportional to increasing diffusion coefficient. As diffusion coefficient increases the concentration of contaminant increases.EM schemes above from fig. 2 have higher effects of concentration of contaminants as D increases compared to other schemes.The concenttation of contaminants increases with increase in flow velocity.MOL values shows that there is general nonlinear increase of concentration of contaminants as D increases beacause of truncation errors due to discretization of space variable and round off errors from the solver.Generally,an increase in diffusion coeffients produces an increase in concentration of contaminants and also portray that small values of D has more effect on concentration of contaminant that larger value of diffusion coefficient.

4.3 Results and discussion of objective 3

The following data is used: D = 0.1,μ= 0.8m/s at t = 1s.The concentration are taken from the analytical solutions and scheme by (Dehghan 2005).The numerical scheme are presented using uniform grid, under a mesh of width Δx = 0.1m, data is presented in figure 3 to compare the accuracy of the numerical methods with analytical solution.

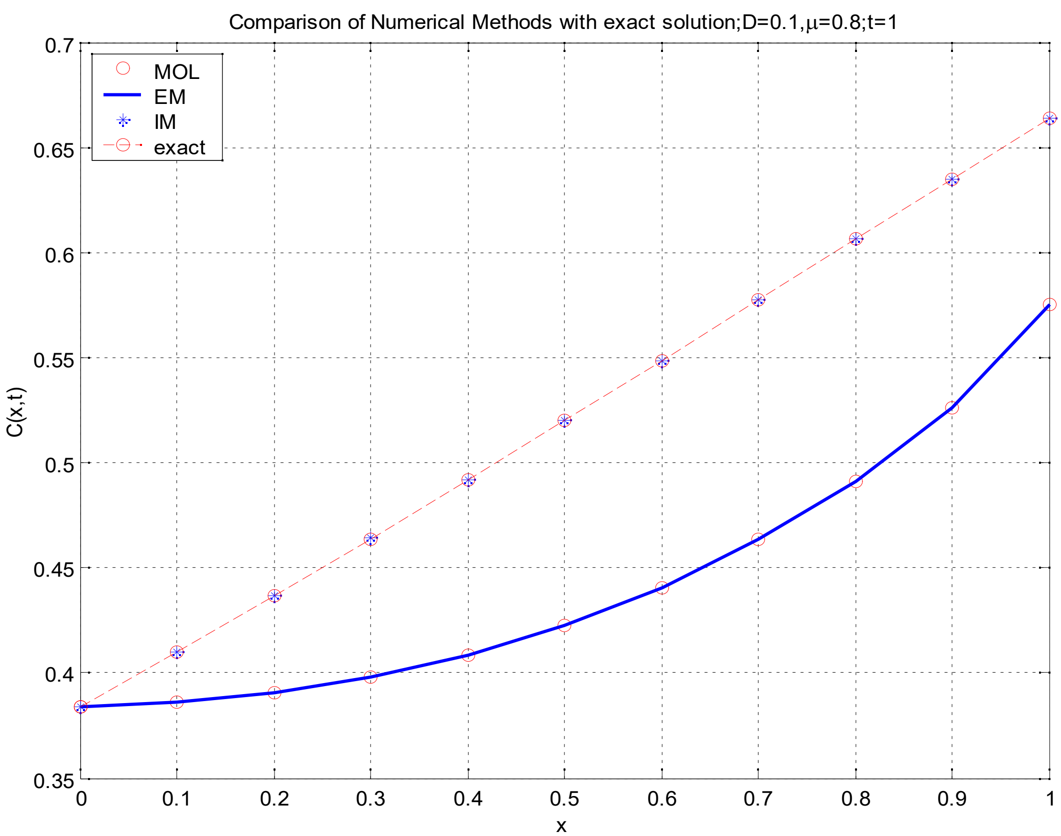


Figure 3: Comparison of numerical methods used with exact method analysis.

The errors of method values of concentration above clearly shows there is the implicit method coincided with exact solution due unconditionally stabilities while method of lines coincided with explicit method which is conditionally stable thus shows that implicit method is most accurate than EM and MOL scheme.

CHAPTER FIVE

CONCLUSION AND RECOMMENDATION

5.1: Introduction

This chapter presented conclusions and suggestions on recommendations for further study by newly researchers on convection diffusion equations.

5.2: Conclusion

The study successfully implemented and developed numerical simulations using Implicit Backward Euler method (IM), explicit method (EM) and Methods of Line (MOL) schemes from finite difference method (FDM). Generally the methods showed the following effects;

i) As the velocity of the flow increases the concentration of the contaminants decreases

ii) As the diffusion coefficient increases the concentration of contaminants increases

iii) Implicit method is most accurate method than explicit method and method of lines scheme due it has coincided with exact method scheme.

5.2: Recommendations

Others researchers may study the following recommendations;

(i) The effect of Reynolds number on the concentration of contaminants

(ii) Use of Finite Elements Methods (FEM) can be utilized for simulation

(iii) Study the effect of the parameters studied on a 2D – Case

i.e. $C_t + \mu_1 C_x + \mu_2 C_y = D_1 C_{xx} + D_1 C_{yy}$

(iv) Use Operator Splitting Method can be utilized for simulation

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APPENDIX I: DATA VALUES FOR OBJECTIVE ONE

The appendix 1 show the data of numerical schemes presented in table a, b and c for objective one obtained from equation 1.2b,3.1.9,3.2.8 and 3.3.5 respectively for analysis

Table a: Exact, Implicit, Explicit and MOL values of C (mg/l); D=0.1; t=1, for $\mu = 0.8m/s$

Length , x (m)	Exact method	Explicit method	Implicit method	MOL
	C (mg/l)			
0	0.3838	0.5764	0.3838	0.3838
0.1	0.4097	0.6578	0.4098	0.3862
0.2	0.4364	0.6952	0.4366	0.3907
0.3	0.4637	0.7264	0.4640	0.3978
0.4	0.4916	0.7540	0.4919	0.4081
0.5	0.5199	0.7816	0.5202	0.4225
0.6	0.5485	0.8079	0.5488	0.4406
0.7	0.5773	0.8319	0.5776	0.4636
0.8	0.6062	0.8513	0.6064	0.4908
0.9	0.6350	0.8616	0.6352	0.5258
1	0.6636	0.8581	0.6636	0.5751

Table b: Exact, Implicit, Explicit and MOL values of C (mg/l); D=0.1; t=1, for $\mu = 0.9m/s$

Length ,x (m)	Exact method	Explicit method	Implicit method	MOL
	C (mg/l)			
0	0.3586	0.5794	0.3586	0.3586
0.1	0.3838	0.6549	0.3839	0.3601
0.2	0.4097	0.6922	0.4099	0.3630
0.3	0.4364	0.7225	0.4367	0.3679
0.4	0.4637	0.7512	0.4641	0.3756
0.5	0.4916	0.7789	0.4919	0.3868
0.6	0.5199	0.8054	0.5203	0.4019
0.7	0.5485	0.8298	0.5489	0.4216
0.8	0.5773	0.8500	0.5776	0.4467
0.9	0.6062	0.8619	0.6064	0.4802
1	0.6350	0.8605	0.6350	0.5323

Table c: Exact, Implicit, Explicit and MOL values of C (mg/l); D=0.1; t=1, for $\mu = 1\ m/s$

Length, x (m)	Exact method	Explicit method	Implicit method	MOL
	C (mg/l)			
0	0.3343	0.5824	0.3343	0.3343
0.1	0.3586	0.6521	0.3587	0.3351
0.2	0.3838	0.6892	0.4099	0.3369
0.3	0.4097	0.7195	0.4367	0.3402
0.4	0.4364	0.7483	0.4641	0.3456
0.5	0.4637	0.7762	0.4919	0.3538
0.6	0.4916	0.8028	0.5203	0.3657
0.7	0.5199	0.8276	0.5489	0.3820
0.8	0.5485	0.8486	0.5776	0.4039
0.9	0.5773	0.8620	0.6064	0.4352
1	0.6062	0.8628	0.6350	0.4885

APPENDIX II: DATA VALUES FOR OBJECTIVE TWO

Table a: Exact, Implicit, Explicit and MOL values of C (mg/l);$\mu = 0.8$ m/s, t=1, for $D = 0.1$

Length, x (m)	Exact method	Explicit method	Implicit method	MOL
	C (mg/l)			
0	0.3838	0.6041	0.3838	0.3838
0.1	0.4097	0.6393	0.4097	0.3862
0.2	0.4364	0.6693	0.4364	0.3907
0.3	0.4616	0.6991	0.4616	0.3978
0.4	0.4916	0.7284	0.4916	0.4081
0.5	0.5199	0.7570	0.5199	0.4225
0.6	0.5485	0.7848	0.5485	0.4406
0.7	0.5773	0.8116	0.5773	0.4636
0.8	0.6062	0.8371	0.6062	0.4908
0.9	0.6350	0.8611	0.6350	0.5258
1	0.6636	0.8806	0.6636	0.5751

Table b: Exact, Implicit, Explicit and MOL values of C (mg/l), $\mu = 0.8\ m/s$, t=1, for $D = 0.2$

Length, x (m)	Exact method	Explicit method	Implicit method	MOL
	C (mg/l)			
0	0.6120	0.7771	0.6120	0.6120
0.1	0.6323	0.7992	0.6324	0.6159
0.2	0.6526	0.8180	0.6526	0.6212
0.3	0.6727	0.8360	0.6727	0.6281
0.4	0.6926	0.8534	0.6926	0.6368
0.5	0.7123	0.8700	0.7123	0.6475
0.6	0.7316	0.8858	0.7316	0.6606
0.7	0.7506	0.9007	0.7506	0.6767
0.8	0.7691	0.9148	0.7691	0.6966
0.9	0.7872	0.9278	0.7872	0.7223
1	0.8047	0.9383	0.8047	0.7567

Table c: Exact, Implicit, Explicit and MOL values of C (mg/l) , $\mu = 0.8 m/s$ t=1, for $D = 0.3$

Length, x (m)	Exact method	Explicit method	Implicit method	MOL
	C (mg/l)			
0	0.7150	0.8452	0.7150	0.7150
0.1	0.7308	0.8610	0.7307	0.7189
0.2	0.7463	0.8746	0.7463	0.7239
0.3	0.7615	0.8874	0.7615	0.7299
0.4	0.7765	0.8996	0.7765	0.7372
0.5	0.7911	0.9112	0.7911	0.7461
0.6	0.8054	0.9222	0.8053	0.7567
0.7	0.8192	0.9326	0.8192	0.7695
0.8	0.8327	0.9423	0.8326	0.7850
0.9	0.8457	0.9511	0.8456	0.8042
1	0.8582	0.9583	0.8582	0.8281

APPENDIX III: DATA VALUES FOR OBJECTIVE THREE

Table 3: Errors of methods D=0.1; μ=0.8; t=1

x	Exact	Explicit	Explicit Error	Implicit	Implicit Error	MOL	MOL Error
0.00	0.3838	0.3838	0.0000	0.3838	0.0000	0.3838	0.0000
0.10	0.4097	0.3862	0.0235	0.4098	0.0001	0.3862	0.0235
0.20	0.4364	0.3907	0.0457	0.4366	0.0002	0.3907	0.0457
0.30	0.4637	0.3978	0.0659	0.4640	0.0003	0.3978	0.0659
0.40	0.4916	0.4081	0.0835	0.4919	0.0003	0.4081	0.0835
0.50	0.5199	0.4225	0.0974	0.5202	0.0003	0.4225	0.0974
0.60	0.5485	0.4406	0.1079	0.5488	0.0003	0.4406	0.1079
0.70	0.5773	0.4636	0.1137	0.5776	0.0003	0.4636	0.1137
0.80	0.6062	0.4908	0.1154	0.6064	0.0002	0.4908	0.1154
0.90	0.6350	0.5258	0.1092	0.6352	0.0002	0.5258	0.1092
1.00	0.6636	0.5751	0.0885	0.6636	0.0000	0.5751	0.0885

APPENDIX IV: SIMILARITYREPORT

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